Computing Gröbner Bases of Ideals of Few Points in High Dimensions

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Abstract

A contemporary and exciting application of Gröbner bases is their use in computational biology, particularly in the reverse engineering of gene regulatory networks from experimental data. In this setting, the data are typically limited to tens of points, while the number of genes or variables is potentially in the thousands. As such data sets vastly underdetermine the biological network, many models may fit the same data and reverse engineering programs often require the use of methods for choosing parsimonious models. Gröbner bases have recently been employed as a selection tool for polynomial dynamical systems that are characterized by maps in a vector space over a finite field.

While there are numerous existing algorithms to compute Gröbner bases, to date none has been specifically designed to cope with large numbers of variables and few distinct data points. In this paper, we present an algorithm for computing Gröbner bases of zero-dimensional ideals that is optimized for the case when the number m of points is much smaller than the number n of indeterminates. The algorithm identifies those variables that are *essential*, that is, in the support of the standard monomials associated to a polynomial ideal, and computes the relations in the Gröbner basis in terms of these variables. When n is much larger than m, the complexity is dominated by nm^3. The algorithm has been implemented and tested in the computer algebra system *Macaulay 2*. We provide a comparison of its performance to the Buchberger-Möller algorithm, as built into the system.

Keywords: Gröbner bases, Buchberger-Möller algorithm, essential variables, run-time complexity, computational biology applications

1 Introduction

The theory of Gröbner bases has been an active field of study in the last four decades, beginning with the seminal work of Buchberger [6]. A problem of particular interest has been the development of algorithms for computing Gröbner bases. The first algorithm, proposed by Buchberger, has time complexity that is doubly exponential in the number of variables [7]. Since then, several improvements to Buchberger's algorithm have been proposed, as well as a number of alternative methods for certain classes of ideals.

Many of the improvements focus on two aspects. The first is coefficient growth when computing Gröbner bases in a field of characteristic 0 (for example, see [5]). The second is Buchberger's Criterion, which states that

> "A set $G = \{g_1, \dots, g_r\} \subset I$ is a Gröbner basis for I if and only if the S-polynomial $\overline{S(g_i, g_j)}^G$ is 0 for all $1 \leq i, j \leq r$."

The Optimized Buchberger Algorithm [9] proposed by Caboara *et al.* and Faugére's $F4$ and $F5$ [13, 14] are instances of methods that seek to minimize the number of S-polynomials to be computed. While they still have exponential complexity in the worst case, in practice their performance renders them efficient alternatives to the original Buchberger algorithm.

For zero-dimensional ideals, several methods have been described and implemented. In [8], the authors presented the Buchberger-Möller algorithm (BMA) for computing the reduced Gröbner basis for the vanishing ideal of a variety V over a field. This algorithm eliminates the need to compute S-polynomials and instead performs Gaussian elimination on a generalized Vandermonde matrix. Its complexity is quadratic in the number of variables and cubic in the number of points in V (for details, see [20, 21, 22]). It has been implemented in publicly available computer algebra systems such as CoCoA [10] and *Macaulay 2* [15]. The BMA was later generalized to noncommutative rings [4]. Abbott *et al.* [1] described a modular version of the BMA for the case when $k = \mathbb{Q}$.

There are other algorithms for zero-dimensional ideals which have been developed for particular settings. Farr and Gao presented an algorithm based on a generalization of Newton interpolation in [12]. While the complexity is exponential in the number n of variables, the algorithm has been optimized for the case in which n is small as compared to the number of points. Lederer proposed a method for lexicographic term orders which gives insight into the structure of the Gröbner basis [19].

A recent and exciting development in the theory of Gröbner bases is their use in computational biology. For instance they have been used in the identification of critical points of maximum likelihood functions in phylogenetic-tree reconstruction [16]. Gröbner bases have also been employed as a selection tool for polynomial dynamical systems (PDSs) in the study of gene regulatory networks [18] and protein signal transduction networks [3].

In applications to molecular biology, networks often consist of n biochemicals, such as gene products or metabolites, with changing concentration levels. In [18] a method was proposed to reverse engineer biochemical networks, where the levels are mapped to a finite field $k = \mathbb{F}_p$ for some prime p. In this setting, networks are modeled as PDSs, which generalize the widely studied Boolean networks (see [17] for an introduction). Concentration levels are recorded in a vector in k^n, and the data consists of input-output pairs $(s_i, s_{i+1}) \in k^n \times k^n$, where s_i is a vector describing the state of the network at time i, for $i = 1, \ldots, m$. The input vectors can be viewed as an affine variety $V \subset k^n$, and a family of models represented as PDSs is constructed in terms of the vanishing ideal of V. Gröbner bases are then used to select the most parsimonious PDS from this collection. In these applications, the number n is typically in the hundreds to thousands, whereas the number m is at best on the order of tens of measurements.

Below we describe an algorithm for computing Gröbner bases for zero-dimensional ideals (*i.e.*, vanishing ideals) in a polynomial ring R. This algorithm is specialized for the case when the number m of distinct points is much smaller than the number n of variables. In this setting, there are few relations in terms of *essential* variables, that is, variables that are in the support of the standard monomials associated to an ideal. The remaining ones are of the type $x_i - g$ where the leading term x_i is not an essential variable and the support of g has only essential variables. Therefore computation of a Gröbner basis can be restricted to a proper subring of R containing only essential variables. The algorithm identifies these variables and computes relations of the first type using the BMA. The relations of type $x_i - g$ are computed using standard linear algebra techniques. We have implemented the algorithm, which we call EssBM, in *Macaulay 2*.

The paper is organized as follows. First we describe the EssBM algorithm. In Section 3, we provide the theoretical support for the algorithm and include a complexity analysis. In Section 4, we compare its performance to the BMA, as implemented in *Macaulay 2*. We conclude our paper with a discussion of future directions.

2 The EssBM Algorithm

Let $R = k[x_1, \ldots, x_n]$ where k is a field, and $\succeq$ be a fixed term order on R. Consider a variety $V \subset k^n$ of points with multiplicity one and $|V| = m < \infty$. Here we are primarily interested in finite fields, where these conditions will automatically be satisfied for all varieties. The goal of the EssBM algorithm is to construct the reduced Gröbner basis G with respect to $\succeq$ for the ideal $\mathbf{I}(V)$ of points in V and the set $\mathfrak{B}(G)$ of standard monomials associated to G, which forms a basis for the k-vector space $R/\mathbf{I}(V)$. The algorithm constructs a set $EV \subset \{x_1 \ldots, x_n\}$ of *essential variables*, a set SM of monomials on $\{x_1 \ldots, x_n\}$, and subsets GB and Rel of the ring R. We will see below that G will be given by $GB \cup Rel$ and $\mathfrak{B}(G)$ by the set SM. The *support* (defined in the next section) of the elements in SM is the set EV. We let EV_i, SM_i, GB_i, and Rel_i denote the i-th approximations of the corresponding sets.

Initialize each set as follows: $EV_0 = \{\}$, $SM_0 = \{1_R\}$, $GB_0 = \{\}$, and $Rel_0 = \{\}$. Let $[n]$ denote the set $\{1, \ldots, n\}$ and x^a the monomial $x_1^{a_1} \cdots x_n^{a_n}$. For each $i \in [n]$, do the following. Find the i-th smallest variable, say x_i. Suppose there are r monomials $x^{a_1}, \ldots, x^{a_r}$ in SM_{i-1} that are smaller than x_i in the given ordering. Try to write x_i as a k-linear combination of these monomials. That is, find (if they exist) $c_1, \ldots, c_r \in k$, where

$$\begin{aligned} x_i(1) &= \sum_{j=1}^{r} c_j x^{a_j}(1) \\ x_i(2) &= \sum_{j=1}^{r} c_j x^{a_j}(2) \\ &\cdots \\ x_i(m) &= \sum_{j=1}^{r} c_j x^{a_j}(m) \end{aligned} \qquad (1)$$

and $x^a(t)$ is the evaluation of x^a at the t-th point in V for $t \in [m]$. If there are such coefficients, then

$$x_i(t) - \sum_{j=1}^{r} c_j x^{a_j}(t) = 0$$

for every $t \in [m]$ and it follows that $h := x_i - \sum_{j=1}^{r} c_j x^{a_j} \in \mathbf{I}(V) \cap k[EV_{i-1} \cup \{x_i\}]$, where $k[EV_{i-1} \cup \{x_i\}]$ is the polynomial ring in the variables in $EV_{i-1} \cup \{x_i\}$. Since the monomials x^{a_j} were chosen so that $x_i \succeq x^{a_j}$, it follows that x_i is the leading term of an element of $\mathbf{I}(V)$ and so is not a standard monomial. In this case let $Rel_i = Rel_{i-1} \cup \{h\}$. If there is no solution to the system in (1), then x_i is a standard monomial. In this case let $EV_i = EV_{i-1} \cup \{x_i\}$, and compute the Gröbner basis GB_i and the set SM_i of standard monomials for the ideal $\mathbf{I}(V) \cap k[EV_i]$ of the points projected onto the variables in EV_i. When $i = n$, return the sets $G := GB_n \cup Rel_n$ and $\mathfrak{B}(G) := SM_n$.

Below we give pseudo-code for the complete algorithm, which has been implemented in *Macaulay 2*. While the BMA computes *separators* for the points in V in addition to the Gröbner basis and the set of standard monomials, the implementation in *Macaulay 2* does not. In order to appropriately compare the two implementations, we do not include separators in this version of EssBM. However, our algorithm can easily be modified to return the separators at an additional cost of $O(m)$.

For simplicity, let $[x_j(t)]_{t=1}^{m}$ denote the $(m \times 1)$-column vector

$$\begin{pmatrix} x_j(1) \\ x_j(2) \\ \vdots \\ x_j(m) \end{pmatrix}.$$

The EssBM Algorithm

Input: V a variety; $\succeq$ a term order
Output: G the reduced Gröbner basis for $\mathbf{I}(V)$ with respect to $\succeq$;
$\mathfrak{B}(G)$ the set of standard monomials for G

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Initialize: $EV_0 := \{\}$;  $SM_0 := \{1_R\}$;  $GB_0 := \{\}$;  $Rel_0 := \{\}$.
For $i$ from 1 to $n$ do
    $x_i :=$ $i$-th smallest variable
    $S := k[EV_{i-1} \cup \{x_i\}]$ with term order $\succeq_S$ induced by $\succeq$
    $r := |SM_{i-1}|$ and $LM_i := \{x^{a_j} \preceq_S x_i : x^{a_j} \in SM_{i-1}, 1 \leq j \leq r\}$ the standard monomials less than $x_i$
    $A_i := (m \times (s+1))$-matrix with $s = |EV_{i-1}|$
    first column $[x_i(t)]_{t=1}^{m}$   and   $s$ columns $[x_j(t)]_{t=1}^{m}$ for all $x_j \in EV_{i-1}$
    $Eval_i := (m \times r)$-matrix $(x^{a_j}(p_t))$, where $x^{a_j} \in LM_i$ is evaluated on $p_t$, the point in row $t$ of $A_i$
    If there is a solution $c = (c_1, \ldots, c_r)^T$ to the system of linear equations $Eval_i \cdot c = [x_i(t)]_{t=1}^{m}$
        then $Rel_i := Rel_{i-1} \cup \{x_i - \sum c_j x^{a_j}\}$ where $x^{a_j} \in LM_i$
        else $EV_i := EV_{i-1} \cup \{x_i\}$ and compute $GB_i$ and $SM_i$ in $k[EV_i]$ using the BMA on $A_i$
Return $G = GB_n \cup Rel_n$ and $\mathfrak{B}(G) = SM_n$
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The variables in EV_n are called *essential*. The polynomial $x_i - \sum c_j x^{a_j}$ computed in the i-th step of the algorithm has x_i as its leading term since the monomials x^{a_j} were chosen to be smaller than x_i. The variables x_i are called *inessential* since they can be written in terms of essential variables.

3 Theoretical Background

In this section, we provide a detailed proof of the correctness and worst-case time complexity of the EssBM algorithm. Before stating and proving the main results, namely Theorems 5, 7 and 8, we begin with some preliminaries.

Recall that the matrix A_i has rows corresponding to the points in V projected onto the coordinates defined by $EV_i = EV_{i-1} \cup \{x_i\}$. Let P_i be this set of projected points.

For the remainder of this paper, we use the shorthand notation I for the ideal $\mathbf{I}(V)$ and $k[EV_i]$ for the polynomial ring in the variables in the set EV_i. Also, we let $G = GB_n \cup Rel_n$ and $\mathfrak{B}(G)$ the set of standard monomials for G.

Lemma 1. *The equality $\mathbf{I}(P_i) = I \cap k[EV_i]$ holds.*

Proof. This follows immediately from the construction of the ideal $\mathbf{I}(P_i)$. □

Corollary 2. *The set GB_i is the reduced Gröbner basis for the ideal $I \cap k[EV_i]$ with respect to $\succeq$ and SM_i is the set of standard monomials for $I \cap k[EV_i]$ with respect to GB_i. In particular, the statement holds for $i = n$.*

Proof. The sets GB_i and SM_i are the reduced Gröbner basis and the set of standard monomials, respectively, for the ideal $\mathbf{I}(P_i)$ in $k[EV_i]$. From the previous lemma, we have that $\mathbf{I}(P_i) = I \cap k[EV_i]$. Hence the result follows. □

Let $f \in R$ be a polynomial. We define the *support* of f, denoted by *supp*(f), to be the set of variables that appear in f. By construction, *supp*(f) is the smallest set $X \subset \{x_1, \ldots, x_n\}$ such that $f \in k[X]$. The *support* of a set of polynomials S is the union over the support of each polynomial $g \in S$. Let $LT(f)$ denote the leading term of f with respect to a given term order. The *tail* of f is the polynomial $tail(f) := f - LT(f)$.

Lemma 3. *Let $f \in R$ be such that supp$(f) \subset EV_n \cup \{x_{\beta_1}, \ldots, x_{\beta_s}\}$ where $x_{\beta_1} \prec \cdots \prec x_{\beta_s}$ are inessential variables. Suppose that supp$(LT(f)) \subset EV_n$. Then there is $f^* \in R$ such that supp$(f^*) \subset EV_n \cup \{x_{\beta_1}, \ldots, x_{\beta_{s-1}}\}$, the polynomial f^* has the same leading term as f, and $f - f^* \in I$.*

Proof. Consider the largest inessential variable x_{β_s}. We can write

$$f = LT(f) + \sum_{i=0}^{r} (x_{\beta_s})^i h_i$$

where *supp*$(h_i) \subset EV_n \cup \{x_{\beta_1}, \ldots, x_{\beta_{s-1}}\}$. As x_{β_s} is an inessential variable, there is an element $x_{\beta_s} + g$ of Rel_n with leading term x_{β_s}. Note that *supp*$(g) \subset EV_n$. Define the polynomial f' from f by replacing each $(x_{\beta_s})^i$ with $-(x_{\beta_s})^{i-1}g$:

$$f' = LT(f) - \sum_{i=0}^{r} (x_{\beta_s})^{i-1} g h_i.$$

Then

$$f - f' = \sum_{i=0}^{r} \Big((x_{\beta_s})^i + (x_{\beta_s})^{i-1} g \Big) h_i \in I$$

since $(x_{\beta_s})^i + (x_{\beta_s})^{i-1} g = (x_{\beta_s})^{i-1}(x_{\beta_s} + g) \in I$. As $LT(f) \succ x_{\beta_s} \succ LT(g)$, we have that $LT(f') = LT(f)$. Let f^* be the polynomial obtained after r replacements of x_{β_s}. Note that we have $f - f^* \in I$ and $LT(f^*) = LT(f)$. Since we have replaced all occurrences of x_{β_s}, it follows that *supp*$(f^*) \subset EV_n \cup \{x_{\beta_1}, \ldots, x_{\beta_{s-1}}\}$. □

This lemma gives us a way of removing inessential variables from a polynomial in I without affecting its leading term, which will be useful for proving the correctness of EssBM (Theorems 5 and 7). In fact, we can remove *all* inessential variables. We emphasize this fact with the following corollary.

Corollary 4. *Let $f \in R$. Then there is $f^* \in R$ such that supp$(f^*) \subset EV_n$, $LT(f^*) = LT(f)$, and $f - f^* \in I$.*

Theorem 5. *The set G is the reduced Gröbner basis for I with respect to $\succeq$.*

Proof. We first show that $G \subset I$. Consider $g \in G$. If $g \in GB_n$, then $g \in I$. Suppose that $g \in Rel_n$. Then g is of the form $x_i - \sum c_j x^{a_j}$ for some $c_j \in k$ and $x^{a_j} \in R = k[x_1, \ldots, x_n]$. The coefficients c_j were chosen so that $x_i(t) = \sum c_j x^{a_j}(t)$ for all $t \in [m]$. Therefore by construction $g \in I$.

Now let $f \in I$. We must show that there is some $g \in G$ such that $LT(g) \mid LT(f)$. We distinguish two cases.

Case 1: *supp*$(LT(f)) \not\subset EV_n$.

Suppose that $LT(f)$ contains an inessential variable x_i. By construction of the set Rel_n, there is an element g of $Rel_n \subset G$ with leading term x_i. It follows that $LT(g)$ divides the leading term of f.

Case 2: $supp(LT(f)) \subset EV_n$.

Recall that the set GB_n is a Gröbner basis of the projection of I onto the variables in EV_n (see Corollary 2). If $supp(tail(f))$ is also contained in EV_n, then $f \in k[EV_n]$ and there is a $g \in GB_n \subset G$ whose leading term divides $LT(f)$.

Assume that $supp(tail(f)) \not\subset EV_n$. Using Corollary 4, we can find $h \in I$ such that $supp(f-h) \subset EV_n$ and $LT(f-h) = LT(f)$. Since $f-h \in k[EV_n]$, there is a $g \in GB_n \subset G$ whose leading term divides $LT(f-h) = LT(f)$.

To prove that G is reduced, let $g \neq h \in G$. We wish to show that g and h satisfy the following criterion:

$$LT(g) \text{ does not divide any monomial in } h. \tag{2}$$

We consider the following four cases.

Case 1: $g, h \in GB_n$.

As GB_n is the reduced Gröbner basis for the ideal I projected onto the essential variables, then g, h satisfy (2).

Case 2: $g, h \in Rel_n$.

Let $LT(g) = x_i$ and $h = x_j - \sum_i c_i x^{a_i}$ for $i \neq j$. Note that $supp(h) \subset EV_{j-1} \cup \{x_j\}$. Clearly x_i does not divide x_j. As $supp(tail(h)) \subset EV_n$ and $x_i \notin EV_n$, then x_i does not divide any monomials in $tail(h)$.

Case 3: $g \in GB_n$ and $h \in Rel_n$.

Let $LT(h) = x_i$ for some inessential variable. This will not be divisible by $LT(g)$, which contains at least one essential variable. All other terms x^a of h are standard monomials for the projection of I onto the variables in EV_i; in particular, $supp(x^a) \subset EV_i$. It follows that if $supp(g) \subseteq EV_i$, then $LT(g)$ does not divide any term of h. By Corollary 2, $supp(g)$ contains only essential variables. Thus if $supp(g)$ is not contained in EV_i, then $supp(g)$ must contain a variable x_j with $x_i \prec x_j$. This x_j divides some term x^b of g, and it follows that if $LT(g)$ divides some term x^a of h, then $x_j \preceq x^b \preceq LM(g) \preceq x^a \preceq x_i$, which contradicts the assumption that $x_i \prec x_j$.

Case 4: $g \in Rel_n$ and $h \in GB_n$.

Then $LT(g)$ is some inessential variable, say x_i. However, $supp(h) \subset EV_n$ and so g, h satisfy criterion (2).

□

Next we compute the number of elements in $\mathfrak{B}(G)$ and show the relationship between $\mathfrak{B}(G)$ and the set SM_n.

Lemma 6. *The set $\mathfrak{B}(G)$ has $|V|$ elements.*

The previous lemma is usually stated for algebraically closed fields k and proved with the help of the Strong Hilbert Nullstellensatz (see [11]). We include a proof of the statement for the case where all points have multiplicity one, as is being assumed throughout the paper.

Proof. Suppose $V = \{a_1, \ldots, a_m\}$ and define $I_i := \mathbf{I}(\{a_i\})$. Then $I = \mathbf{I}(\bigcup_{i=1}^m \{a_i\}) = \bigcap_{i=1}^m I_i$, since each point a_i has multiplicity one. Note that each of the ideals I_i is maximal and it follows that they are pairwise comaximal. Consider the quotient ring R/I. By the Chinese Remainder Theorem, there is a ring homomorphism such that

$$R/I \cong R/I_1 \times \cdots \times R/I_m.$$

As each I_i is maximal, then each $R/I_i \cong k$ and it follows that $R/I \cong k^m$, as rings. Further, the quotient ring and k^m can be viewed as k-vector spaces, and the isomorphism can be extended to an isomorphism of vector spaces. Hence, the dimension of R/I as a vector space is $dim_k(R/I) = m$. Since $\mathfrak{B}(G)$ forms a basis for the vector space R/I (Proposition 2.1.6 in [2]), we conclude that $|\mathfrak{B}(G)| = m = |V|$. □

Theorem 7. *The set SM_n is the set of standard monomials for I with respect to G.*

Proof. By Corollary 2, we have that SM_n is the set of standard monomials for the ideal $I \cap k[EV_n]$ with respect to the Gröbner basis GB_n. As V has finitely many points, then $|\mathfrak{B}(G)| = |V|$. Consider a monomial $x^a \in \mathfrak{B}(G)$. If $x^a \notin k[EV_n]$, then it contains an inessential variable, say x_i. As x_i is the leading term of an element in $Rel_n \subset I$, it is not a standard monomial for G, contradicting the assumption that $x^a \notin \mathfrak{B}(G)$. Therefore $x^a \in k[EV_n]$.

By construction, $x^a \notin LT(I)$. Using the set-containment relation

$$LT\left(I \cap k[EV_n]\right) \subset LT(I),$$

it follows that $x^a \notin LT(I \cap k[EV_n])$ and so $\mathfrak{B}(G) \subset SM_n$. To see equality, note that the set P_n of projected points defined by EV_n has at most as many points as V. Then $|SM_n| = |P_n| \leq |V| = m$. Since $\mathfrak{B}(G) \subset SM_n$, it follows that $m = |\mathfrak{B}(G)| \leq |SM_n| \leq m$. Hence $\mathfrak{B}(G) = SM_n$; that is, SM_n is the set of standard monomials for I with respect to G. □

We conclude this section with a complexity analysis of EssBM.

Theorem 8. *The EssBM algorithm terminates and has worst-time complexity $O(nm^3) + O(m^6)$, which is dominated by $O(nm^3)$ when $m \ll n$.*

Proof. We compute the complexity of each step and then provide a summary at the end. Step 1 has complexity $O(1)$. In Step 2, the algorithm enters a loop of length n. Steps 3-8 are executed in each iteration of the loop. They have the following complexities:

Step 3. $O(1)$: Executing this step requires constant time since the variable order, given as part of the declaration of the term order, is maintained in one array.

Step 4. $O(m^2)$: This step may not even be required by all implementations; if required, it involves passing $O(m^2)$ variables to a new object of size $O(m^2)$.

Step 5. $O(m^3)$: As term orders are typically stored as matrices, in this case the term order $\preceq_S$ is a matrix of dimension $O(m^2)$. Determining the order between two monomials of S requires multiplication of a vector of length $O(m)$ by this matrix. So for each monomial $x^a \in SM_{i-1}$, there are at most m^2 operations required for comparing x_i to x^a and there are at most m such monomials.

Step 6. $O(m)$: An $(m \times 1)$-column vector is added to a matrix with columns corresponding to the variables in EV_{i-1}.

Step 7. $O(m^3)$: As there are at most m variables in each monomial and at most m^2 entries in the matrix, the cost of executing this step is $O(m^3)$.

Step 8. $O(m^3)$: Solving a linear system of m equations in $r \leq m$ unknowns requires $O(m^3)$ time.

Step 9 has complexity $O(1)$ and will be executed at most n times.

Since there can be at most m essential variables, Step 10 will be executed at most m times. The complexity of each execution of Step 10 is $O(m^5)$: Updating EV_i is a constant operation. However, computing GB_i and SM_i for the matrix A_i is associated to the cost of calling the BMA, which is quadratic in the number of variables and cubic in the number of points. In this case, the numbers of variables and points are given by the dimensions of A_i. Since both row and column dimensions are bounded above by m, it follows that the complexity of executing this step is $O(m^5)$.

Step 11 has complexity $O(n + m^2)$: Note that there are $O(m^2)$ elements in GB_n (see [20]), $O(n)$ relations in Rel_n, and m monomials in SM_n. So returning these sets requires $O(n + m^2 + m)$ operations.

Hence, we can calculate the total complexity $C(EssBM)$ of the algorithm as follows:

$$\begin{aligned} C(EssBM) &= O(1) + O(n)\left[O(1 + m^2 + m^3 + m + m^3 + m^3 + 1)\right] + O(m)O(m^5) + O(n + m^2 + m) \\ &= O(nm^3) + O(m^6). \end{aligned}$$

When $m \ll n$, then $O(nm^3)$ becomes the dominating term and the above estimate reduces to

$$C(EssBM) = O(nm^3).$$

□

4 Performance of the EssBM Algorithm

To test the performance of our algorithm, we compared its run-time to that of the BMA[1], as implemented in *Macaulay 2*, on randomly generated varieties in k^n. For this analysis, we let the field k be $\mathbb{F}_p$ for $p \in \{3, 17\}$. Since the complexities of the two algorithms depend on m and n, we chose a range of values for these parameters, namely, $m \in \{5, 10, 15\}$ and $n \in \{100, 150, 200, 250, 300\}$. For each set of parameters p, m, and n, we generated 10 varieties using a built-in random number generator in *Macaulay 2*, without specifying prior constraints on the relative position of the points in the variety. We performed this experiment using two term orders: a lexicographic order (*lex*) and a graded reverse lexicographic order (*grevlex*), each with the same variable order.

Figures 1 and 2 show the run-times for the two algorithms for $p = 3$ and $m = 5, 15$. As the run-times for $m = 10$ fall between the $m = 5$ and $m = 15$ settings, we omitted them from the plots. We display the results for all parameters settings in the appendix. The run-times for $p = 17$ are similar.

As a measure of the stability of the run-time data, we computed the *coefficient of variation*, defined to be the ratio of the standard deviation to the mean of the data. For the *grevlex* experiments, this coefficient ranges from

[1] The Buchberger-Möller algorithm has been implemented as the function *points* in the "Points" package of *Macaulay 2* distribution version 0.9.8.

0.004 to 0.2, whereas for the *lex* experiments it ranges from 0.01 to 0.1. Since this implies very low variability of the run-times for fixed p, n, and m, we displayed only mean values in Figures 1 and 2.

The empirical results corroborate our theoretical prediction that for $m \ll n$, the EssBM algorithm outperforms the BMA. For small n, however, we observe that EssBM is slower, which we attribute to the overhead costs associated to multiple calls to the BMA.

5 Discussion

Recently, applications of Gröbner bases as a promising model selection tool in molecular biology have been proposed [3, 18]. These applications require computation of a Gröbner basis for a zero-dimensional ideal $\mathbf{I}(V)$ in a polynomial ring $k[x_1, \ldots, x_n]$, where $|V| = m \ll n$. Previously, no algorithms for computing Gröbner bases optimized for $m \ll n$ had been available. The run-time of the existing implementations was a bottleneck in applications of the methods in [3] and [18] to data sets whose size is of the order typical for biochemical data sets such as microarray data.

The EssBM algorithm presented here goes some way towards alleviating this problem in that it reduces the worst-case complexity, which is $O(n^2m^3)$ for the standard Buchberger-Möller algorithm, to $O(nm^3)$ for $m \ll n$. Our implementation and testing indicate that for a small number of distinct points in general position, EssBM starts outperforming a standard implementation of the BMA when the number of variables exceeds 200. This should make it possible to use the methods of [3] and [18] for analysis of larger data sets than was hitherto possible. Unfortunately, the worst-time complexity estimate $O(nm^3 + m^6)$ of the EssBM algorithm suggests that it may still be infeasible for moderately large m. We are currently working on a related algorithm that would further reduce this complexity.

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Appendix

Figure 1: Run-times averaged over 10 randomly generated varieties for $p = 3$ and *lex*.

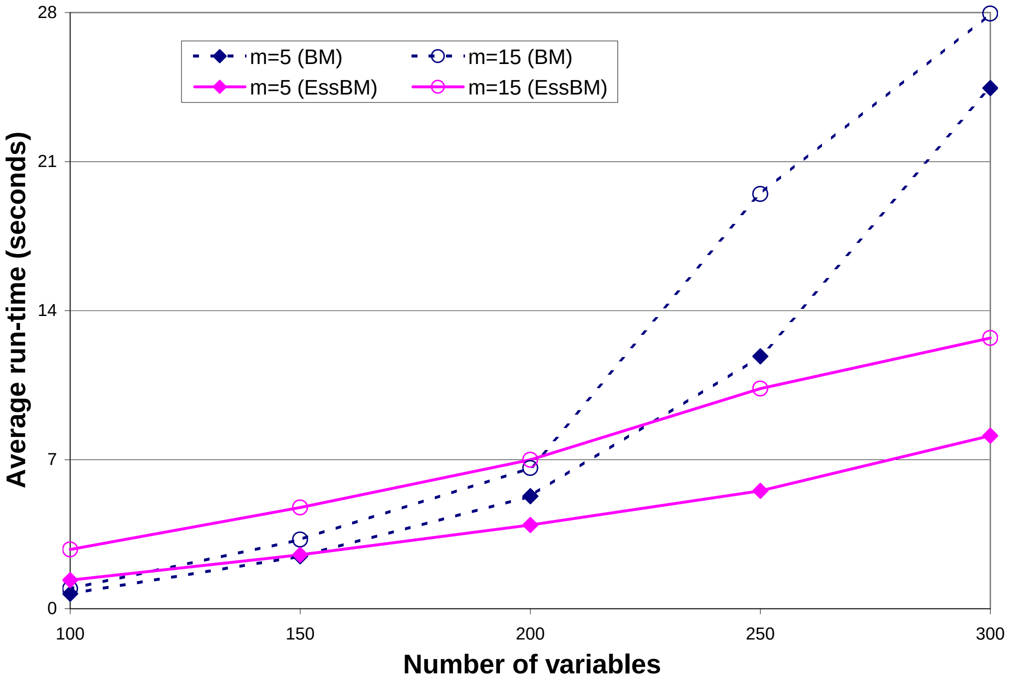


Figure 2: Run-times averaged over 10 randomly generated varieties for $p = 3$ and *grevlex*.

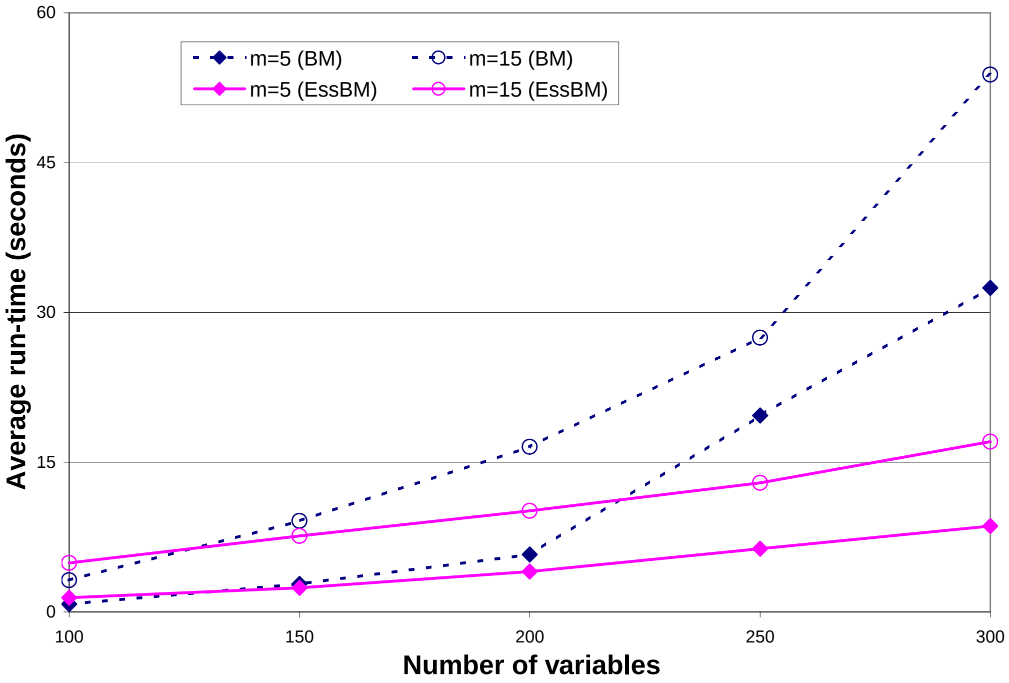


Figure 3: Run-times for 10 randomly generated varieties and *lex*.

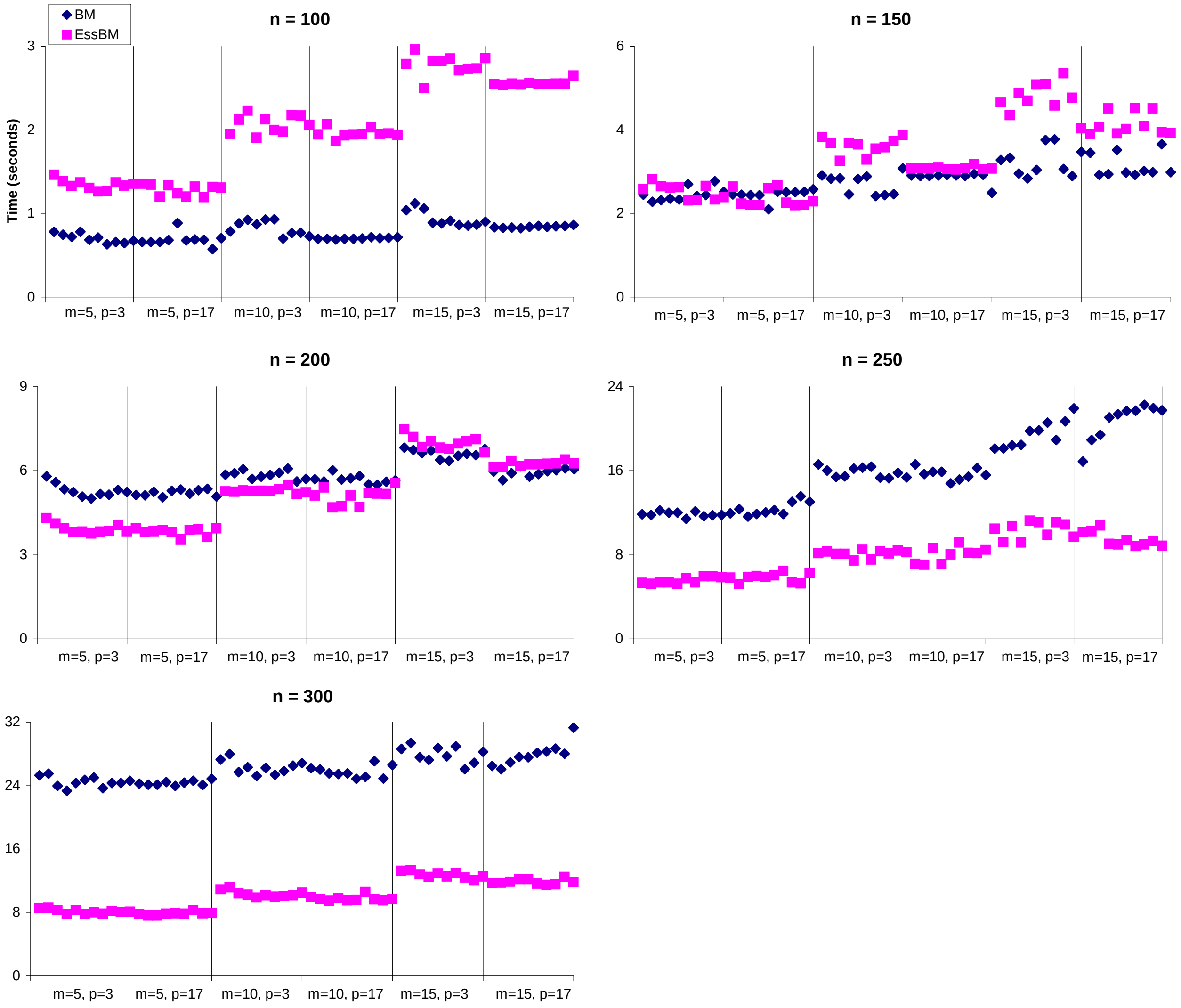
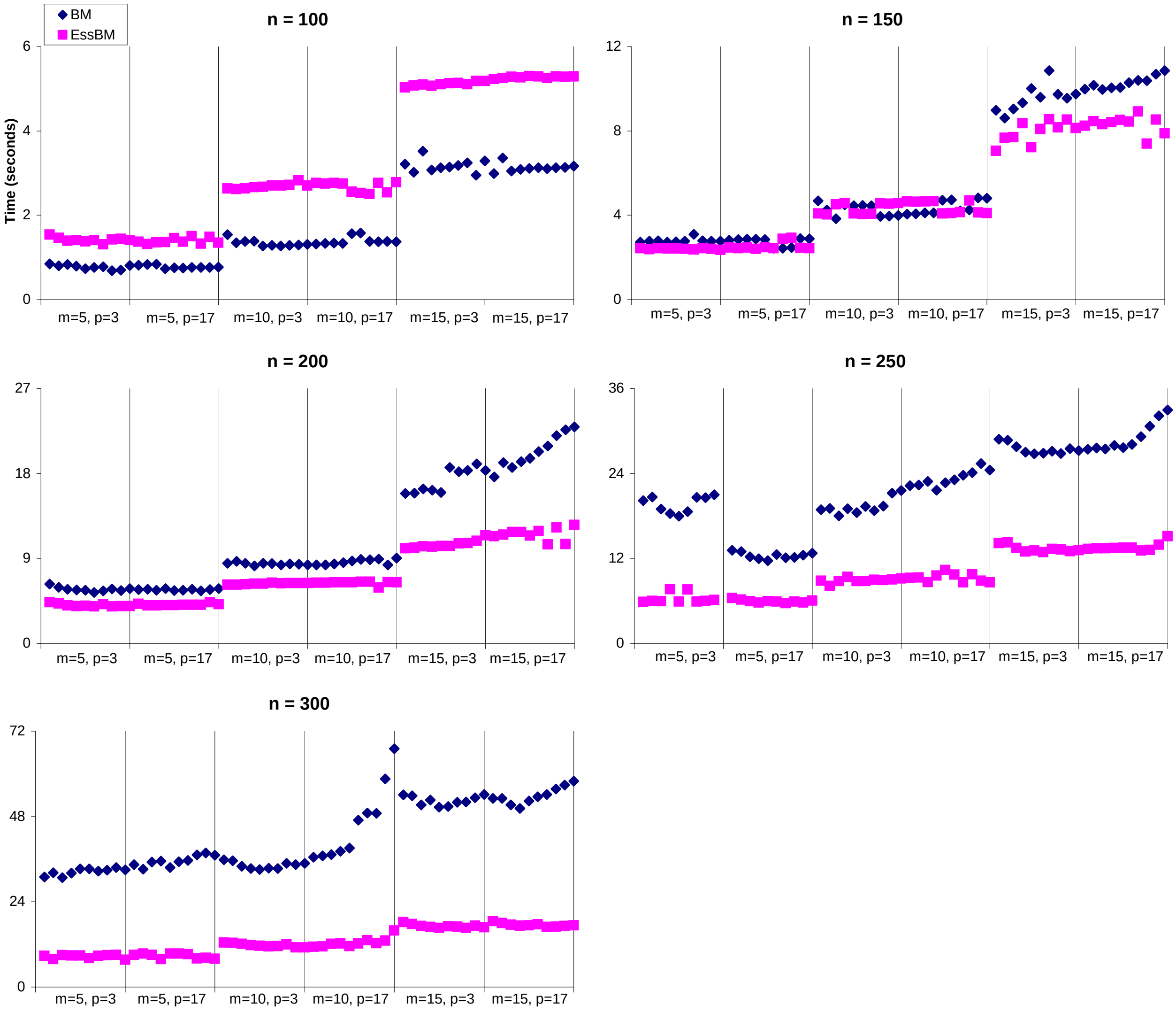


Figure 4: Run-times for 10 randomly generated varieties and *grevlex*.


◆ BM
■ EssBM
n = 100
Time (seconds)
m=5, p=3
m=5, p=17
m=10, p=3
m=10, p=17
m=15, p=3
m=15, p=17
n = 150
m=5, p=3
m=5, p=17
m=10, p=3
m=10, p=17
m=15, p=3
m=15, p=17
n = 200
m=5, p=3
m=5, p=17
m=10, p=3
m=10, p=17
m=15, p=3
m=15, p=17
n = 250
m=5, p=3
m=5, p=17
m=10, p=3
m=10, p=17
m=15, p=3
m=15, p=17
n = 300
m=5, p=3
m=5, p=17
m=10, p=3
m=10, p=17
m=15, p=3
m=15, p=17